First Astronomical Detection of the Carbene Chain H_2C_6

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ABSTRACT

The cumulene carbenes are important components of hydrocarbon chemistry in low mass star forming cores. Here we report the first astronomical detection of the long chain cumulene carbene H_2C_6, in the interstellar cloud TMC1, from observations of two of its rotational transitions: $J_{K,K'} = 7_{17} \rightarrow 6_{16}$ at 18.8 GHz and $8_{18} \rightarrow 7_{17}$ at 21.5 GHz, using NASA's Deep Space Network 70 m antenna at Goldstone, California. In addition we also observed the shorter cumulene carbene, H_2C_4 at the same position. The fractional abundance of H_2C_6 relative to H_2 is about 3×10^{-11} and that of H_2C_4 about 8×10^{-10}. The H_2C_6 abundance is in reasonable agreement with gas phase chemical models for young molecular cloud cores while the H_2C_4 is more abundant than predicted.

Subject headings: interstellar: molecules - line identifications - chemistry; interstellar: molecules - stars: formation

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1. INTRODUCTION

The detection of new cumulene carbenes is important for determining the hydrocarbon chemistry in low mass star forming cores (cf. Bettens & Herbst 1996). The cumulene carbene chains are also of interest in astronomy for their possible role as one of the carriers of the diffuse interstellar bands (McCarthy et al. 1996). Here we report the first astronomical detection of H_2C_6 (hexapentaenylidene) in the dark cloud TMC1. This identification was made possible by the recent laboratory detection of the rotational spectrum of the long chain cumulene carbons, H_2C_5 and H_2C_6 (McCarthy et al. 1996) and the high sensitivity of NASA's Deep Space Network antennas at cm wavelengths.

We also observed the shorter cumulene carbene chains propadienyldene, H_2C_3 (Cernicharo et al. 1991, Kawaguchi et al. 1991), and buttatrienylidene H_2C_4 (Kawaguchi et al.)) at the same position as H_2C_6 to allow comparison to chemical models. H_2C_4 and H_2C_6 have linear carbon backbones anti C_{2v} symmetry, and because of the off-axis equivalent H-atoms have ortho ($K_{\pm 1}$, odd) and para (K_0, even) rotational states, between which both radiative and collisional transitions are highly forbidden. In cold molecular clouds we expect 3/4 of the population to be in the ortho state, and emission from the $K_{\pm 1}$ ladders to be slightly stronger than from the K_0 ladder.

We also observed several other complex molecules in TMC1 to shed light on the hydrocarbon chemistry in star forming cores. We find that the carbon chain molecules vary in abundance among the three principal TMC1 velocity components. The cumulene carbenes are distributed similarly to those of other complex carbon compounds, such as $HC_{2n+1}N$ and C_nH, but differently from the cyclopropenylidene ring c-C_3H_2. We compare the observed ratios to gas phase chemical models appropriate to TMC1.

2. OBSERVATIONS

The observations reported here were made with NASA's Deep Space Network (DSN) 70 meter antenna at Goldstone, CA between October and November of 1996. In addition to H_2C_6 we observed the following species, $HC_9N, C_5H, H_2C_3, H_2C_4$, and c-C_3H_2, as part of an ongoing effort to study complex carbon chemistry in TMC1. We list their relevant transitions and line frequencies in Table 1.

The observations were made with a broad band (17.5 -26 GHz) cooled HEMT receiver with typical system temperatures of 50 - 65 K and the 2 million channel Wide Band Spectrometer Analyzer (WBSA). The spectra were smoothed to resolutions in the range of 0.03 to 0.15 km S-* with a total spectral range of 20 to 40 MHz (cf. Langer et al. 1995).

All the observations except the 18.4 GHz transition of H_2C_6 were made using position switching. In this mode the spectra were obtained by taking the consecutive difference between the ON and OFF source positions every 6 minutes. The right ascension of the OFF source position was also chosen to be 6 minutes in time to the west or east of the ON source position such that each ON-OFF pair had the same mean elevation. This procedure minimizes base line irregularities caused by atmospheric fluctuations. The presence of several stronger lines in the passband of the 21.5 GHz line of H_2C_6 and 20.8 GHz line of H_2C_3 allowed us to check our calibration each observing run. Following our detection of the 21.5 GHz line of H_2C_6 a frequency switching option was implemented for the 1)SN-WBSA system. We used this mode for the observations of the 18.8 GHz transition of H_2C_6 using an LO offset of ().5 MHz between the two frequencies.

The detections reported here were made toward TMC1 at a position RA(1950) = $4^h38^m41^s$ and DEC(1950) = 25 °35'39", corresponding to strongest HC_7N and HC_9N emission as seen in our DSN 70 m high spectral resolution maps (Velusamy et al. 1996), with a reference velocity $V_{lsr} = 5.8$ km s^{-1}. The ON source integration times for the H_2C_6 lines were 23 and 18 hours for the 21.5 and 18.8 GHz transitions, respectively, and yielded a corresponding rms of 2.5 mK and 3.5 mK for spectral resolutions of 0.14 and 0.12 km s^{-1}.

3. RESULTS

In Figure 1 we show the spectra for the two detected transitions of H_2C_6 and for HC_9N, and C_5H. The H_2C_6 2] .5 GHz transition, HC_9N, and C_5H were observed simultaneously in the same passband. The spectrum of $H_2C_4 2_{02} \rightarrow 1_{01}$ at 17.9 GHz in TMC1 is shown in Figure 2, along with the lines of H_2C_3, C_6H, and c-C_3H_2. The H_2C_4 and H_2C_6 spectra peak at ~ 6 km s^{-1} and have peak antenna temperatures, $T_A = 180$ mK and 9 mK, respectively. Previous high spectral resolution studies of complex molecules, such as CCS and HC_7N in TMC1 (Langer et al. 1995) found three velocity components at 5.7, 5.9, and 6.1 km s^{-1} with intrinsically narrow linewidths ~ 0.15 to 0.20 km s^{-1}. Our H_2C_4 spectrum agrees with that of Kawaguchi et al. observed ~ 30" away.

In Figures 1 and 2 it appears that the strongest H_2C_4 and H_2C_6 emission is at 5.9 km S--1. The hint of an asymmetry suggested in these spectra is most likely a second weaker (partially blended) component at 6.1 km s^{-1}, exactly what is seen in the velocity distribution for C_5H and probably C_6H. There is no evidence in H_2C_4 and H_2C_6 for a component at 5.7 km s^{-1}. In contrast the ring molecule c-C_3H_2 and the linear form H_2C_3 show strong emission at 5.7 and 5.9 km s-1, and only slightly less emission at 6.1 km s^{-1}. The presence of strong c-C_3H_2 and H_2C_3 emission at 5.7 km s1 with no evidence of H_2C_6

or H_2C_4 indicates that there is significant chemical inhomogeneity in the hydrocarbons in TMC1 (as is known to be the case for other molecules). Furthermore, the c-C_3H_2 emission is much stronger than that of H_2C_3 ($T_A = 2.0$ K versus 0.12 K).

4.   DIS(3IJSS1ON

To estimate the abundances of H_2C_6 and H_2C_4 in TMC1 we adopted the following simple excitation model in which we treat each ladder as a separate linear rotor. Under molecular cloud conditions the excitation of the ortho and para states of cumulenes can be treated separately because the radiative and collisional transitions between them are negligible. For purposes of estimating abundances the excitation of the ortho ladder can be treated as two single, equivalent linear rotors. The energy levels of the K_+, and K_{-1} ladders are nearly equal and can be estimated within 1% by treating them as a linear rotor with $B_0 = 2(B + C)$ (B and C are given by McCarthy et al.). Collisional rate coefficients for these species have not been calculated; we approximate their J dependent values by using those derived for the linear chain molecule HC_3N (Green and Chapman 1978).

H_2C_6 has a calculated dipole moment of 6.21) (McCarthy et al.) and the J =- 8 ortho levels lie $\sim$ 5 K above the ortho ground state (J = 1). With an Einstein A coefficient of order 2 x 10^{-6} s^{-1} this yields a critical density $n(H_2)$ about 5 x 10^3 cm^{-3}, implying that the lower levels are easily thermalized at the density in the cores of TMC1. Figure 3 shows an excitation calculation for the K_{-1} ortho ladder of H_2C_6 and the K. para ladder of H_2C_4 (using a dipole moment of 4.5])) for a range of fractional abundance gradients (in km s^{-1} pc^{-1}). For convenience the actual calculations were carried out with an existing large velocity gradient (LVG) code which is essentially equivalent to an LTE calculation for optically thin lines, which is almost certainly the case for the weak emission seen in H_2C_4 and H_2C_6. We assumed typical conditions found in the TMC1 clumps: $T_{kin} = 10$ K and $n(H_2) = 10'$ cm^{-3}. The velocity gradient is estimated from the linewidth, ~ 0.3 km s^{-1}, divided by the size of the emission region (from our HC_7N map) $\sim$ 0.06 pc. The total fractional abundances of H_2C_4 and H_2C_6, after accounting for molecules in the other ladders, a velocity gradient of 5 km s^{-1} pc^{-1}, and a beam efficiency of 0.7, are about 1.1 x 10^{-19} and 4.7 x 10-11, respectively. The column density for H_2C_4 derived by Kawaguchi et al. from several transitions at a nearby position corresponds to a fractional abundance of 8 x 10-10 (Bettens et al.) and is in very good agreement with our value. We estimate the abundance ratio of H_2C_4 to H_2C_6 is $\sim$ 25.

' Recent gas phase chemical models have included reaction networks for calculating abundances of large hydrocarbons (Millar et al. 1995, Bettens, Lee & Herbst 1995) and

even very large hydrocarbons (Thaddeus 1994, and Bettens & Herbst 1996). Furthermore, laboratory data and theoretical calculations have begun to shed light on the mechanisms for forming the simplest ring structure cyclopropynylidyne, C-C_3H, via neutral carbon insertion into acetylene, C + C_2H_2 (Kaiser et al. 1996). To compare qualitatively our observations with chemical models we use the results of the gas phase model of Millar et al. (1995), which is based on one of the standard chemical data bases used for modeling cloud chemistry. It includes hydrocarbon production up to 8 or 9 carbons.

In Figure 4 we plot these model abundances for the carbon chains, $C_{2n}H$, $C_{2n+1}H$, H_2C_{2n}, and H_2C_{2n+1}, as well as a point for c-C_3H_2, for the physical conditions relevant to this core of TMC1, $T_{kin} = 10K$ and $n(H_2) = 10^4 cm^{-3}$. Figure 4 shows the early time results of Millar et al. as only this evolutionary stage has enough neutral carbon to produce a successful complex carbon chemistry with large hydrocarbon abundances. The late times, or steady state, solutions have too little carbon and complex carbon species to explain the observations. This result is not surprising as other tracers, such as CCS, confirm the ages of these velocity components to be $\leq$ a few x 10^5 years (Kuiper et al. 1996, Velusamy et al. 1996). Note that the C_nH molecules are predicted to be more abundant than the corresponding H_2C_n molecules, as observed. However, the Millar et al. model also predicts that H_2C_6 is more abundant than H_2C_4 which is exactly the opposite from what we observe. The measured H_2C_6 abundance agrees within a factor of 2 with their model calculations, while the predicted H_2C_4 fractional abundance is too low by a factor $\sim$ 25. We note, however, that the observed H_2C_4/H_2C_6 appears consistent with the slope of the abundance with C_nH.

Bettens et al. explored the effects of various assumptions about the neutral-neutral reactions on the production of complex carbon molecules in interstellar clouds. Bettens and Herbst (1996) recommend using two of these chemical models, the new standard model (NSM) and model 4 (M4), which best explain the polyatomic species. NSM is basically a modified version of the standard ion-molecule chemical scheme while in M4 rapid neutral-neutral reactions play a critical role. A key feature of M4 is that the reactions, O + $C_n \rightarrow C_{n-1} + CO$, for $n > 2$, are assumed negligible. Model M4 of Bettens et al. provides the best agreement with our H_2C_4 observations, but is still too high by a factor of five. The models appear to be sensitive to assumptions about the neutral-neutral reaction rate coefficients at low temperature. H_2C_6 and H_2C_4 are important diagnostics to discriminate among models of hydrocarbon chemistry in dense cores. However, more laboratory measurements and astronomical observations are needed to resolve the hydrocarbon chemistry in star forming cores.

Table 1: Molecular Transitions Observed in TMC1 . . ------ _____

Species	Transition	Rest Frequency MHz	Reference
H_2C_3	1_{01} - 0_{00}	20792.563	Vrtilek et al. "
c-H_2C_3	101 - 0_{00}	**18343.143**	Pickett et al.
H_2C_4	2_{02} - 1_{01}	17863.820	Killian et al.
C_5H	J=9/2 - 7/2 F=5-4b	21484.710	Lovas
C_5H	J=7/2 - 7/2 F=4-3b	214 S5.262	1,ovas
C_6H	J=15/2 - 13/2 F= 8-7	20792.872	Lovas
H_2C_6	7_{17}- $6 1^6$	18802.237	McCarthy et al.
H_2C_6	818-717	2148s.2%	McCarthy et al,
HC_9N	37- ›36	21498.181	Pickett et al.

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Fig. 1--- DSN 70 m detections of H_2C_6 at 21.5 and 18.8 GHz in TMC1. The spectra for H_2C_6 at 21.5 GHz, HC_9N, and C_5H, were all taken within the same passband, while the H_2C_6 18.8 GHz line was observed separately. The source position is $RA(1950) = 4^h38^m41^s$ and $DEC(1950) = 25°35'39"$, with $V_{lsr} = 5.8$ km s^{-1}. The vertical line marks 5.9 km s^{-1}.

Fig. 2.- The spectrum for' H_2C_4 towards TMC1 is shown along with those of H_2C_3, c-C_3H_2, and C_6H. The position is the same as in Figure 1. The vertical line marks 5.9 km s^{-1}.

Fig. 3- The antenna temperatures for the ortho levels of H_2C_6 (solid lines) and para levels of H_2C_4 (dashed lines) calculated using a LVG excitation model and approximating the energy levels with a simple linear rotor (see text) as a function of J. The parameters are $T_{kin} =$ I OK, $n(H_2) = 10^4$ cm^{-3}, and $\Delta V/\Delta L = 1$ km S^{-1} pc^{-1}. Curves for three fractional abundances (in units of km S^{-*} pc^{-1}) are shown for each molecule. The observed T_A for H_2C_4 (filled triangle) and H_2C_6 (filled circles) are marked in the figures along with their 1o error bars. Total fractional abundances need to include a factor for the ortho and para fractions, and the velocity gradient.

Fig. 4.-   The fractional abundances of four carbon chains, $C_{2n}H$, $C_{2n+1}H$, H_2C_{2n+1}, and H_2C_{2n} (solid lines), as a function of n. These are taken from the early time solutions for the gas phase chemical model of Millar et al. for a cold cloud core with $T_{kin} =$ 10K and $n(H_2) = 10^4$ cm^{-3}. The observed fractional abundances of H_2C_4 and H_2C_6, assuming $\Delta V/\Delta L$ $= 5$ km s^{-1} pc^{-1}, are marked by filled boxes.

Figure 1
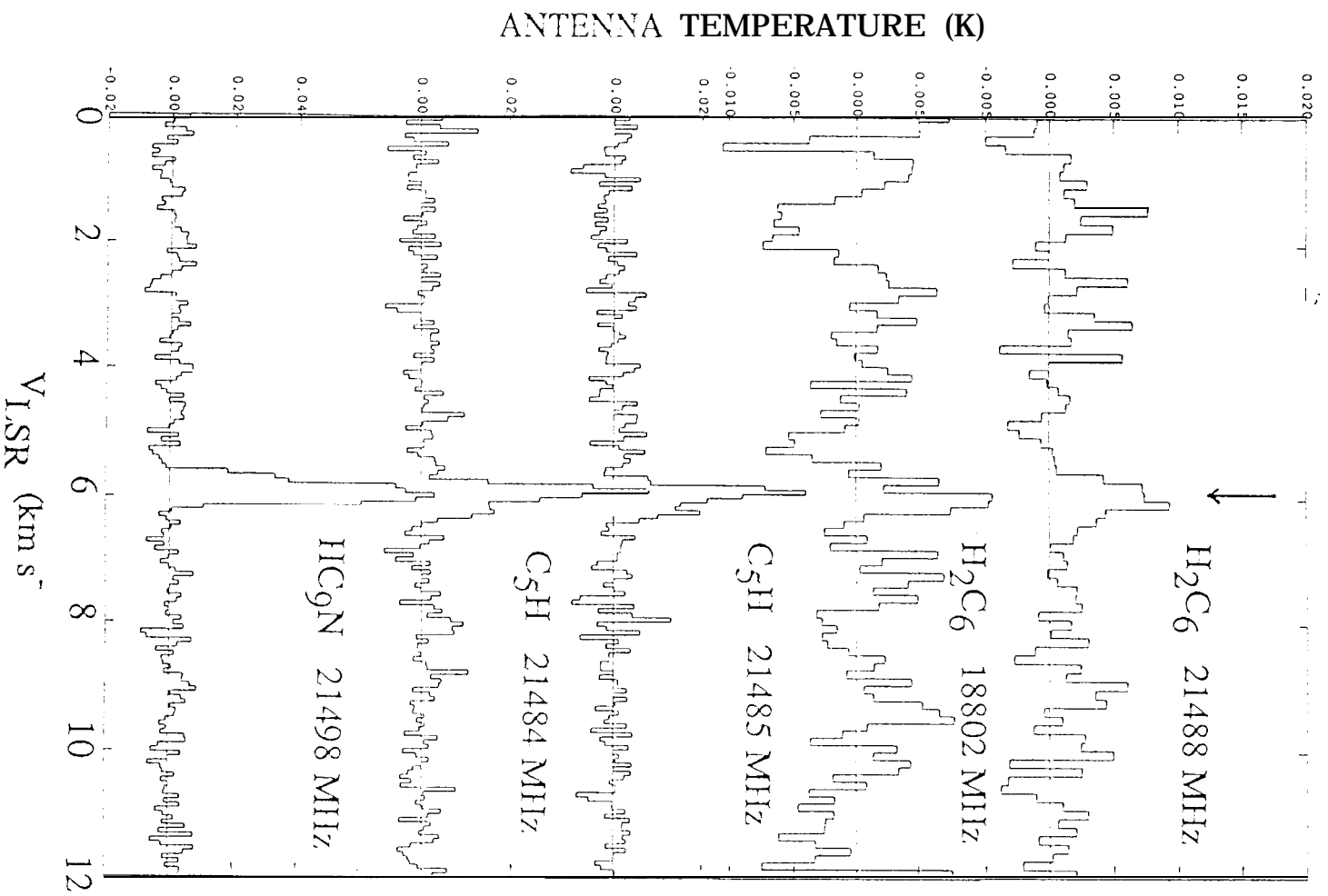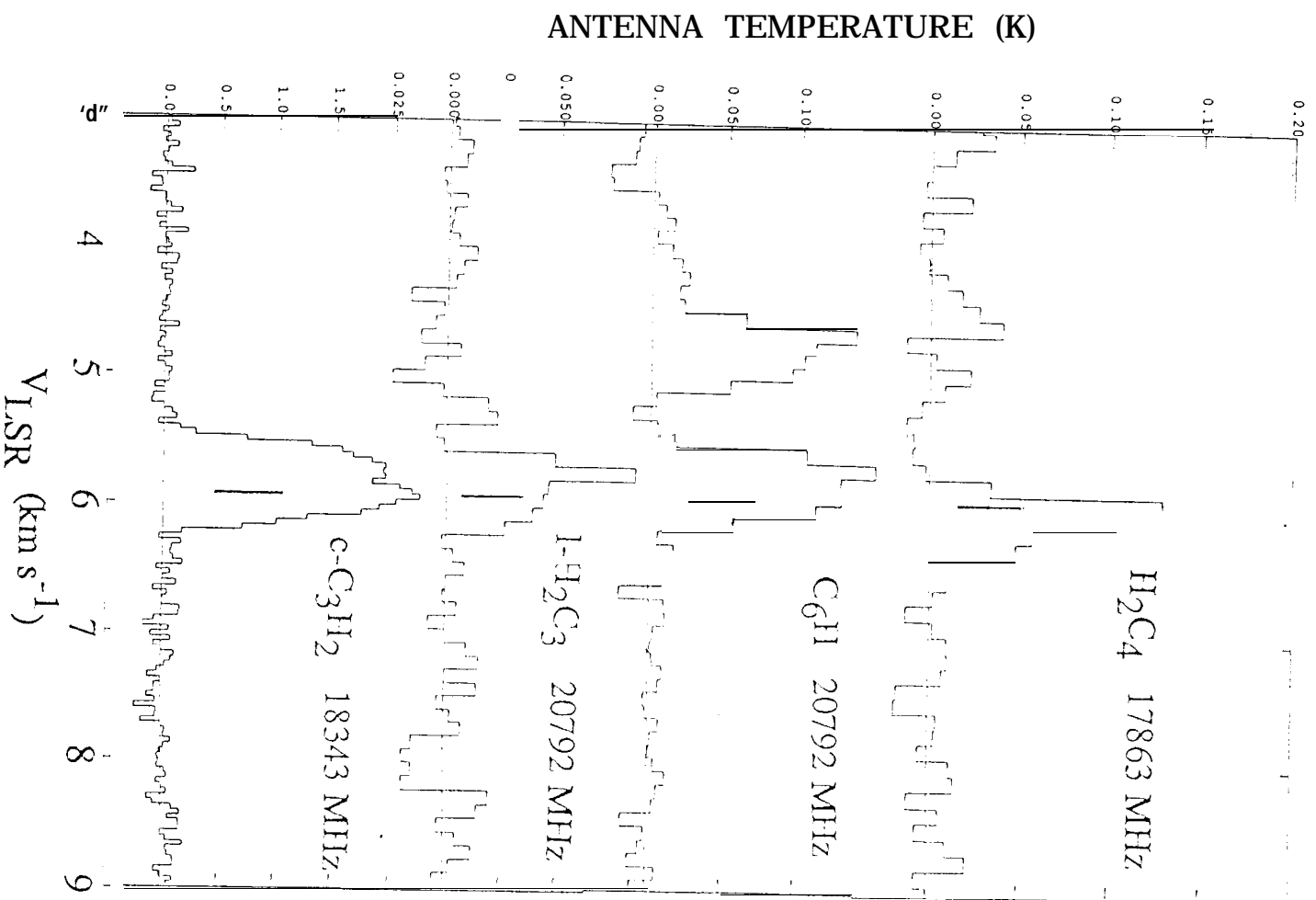
ANTENNA TEMPERATURE (K)
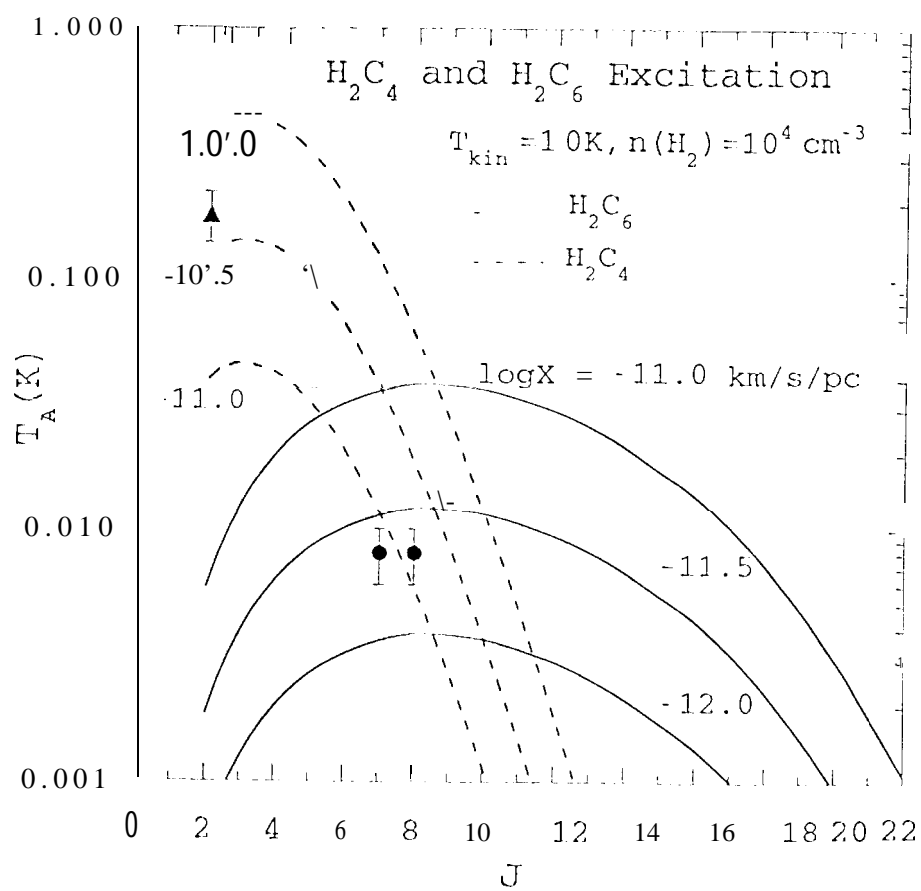
V_{LSR} (km s$^-$)

H_2C_6 21488 MHz

H_2C_6 18802 MHz

C_5H 21485 MHz

C_5H 21484 MHz

HC_9N 21498 MHz

ANTENNA TEMPERATURE (K)

H2C4 17863 MHz.

C6H 20792 MHz.

l-H2C3 20792 MHz.

c-C3H2 18343 MHz.

VLSR (km s⁻¹)

Figure 2

Figure 3

Hydrocarbon Abundances